

Detection of TiH_2 molecule in the interstellar medium is less probable

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Identification of TiH^1 and TiO^2 has been historical, as the Titanium was first time discovered in the interstellar medium (ISM). After finding TiO_2^3 , there is an obvious question about the search of titanium dihydride (TiH_2). The existence of TiH_2 in the ISM is quite probable, as the atomic abundance of hydrogen is about 1900 times larger than that of oxygen. We have discussed that the detection of TiH_2 in the ISM is less probable, though it has a large electric dipole moment.

For analyzing spectrum from the ISM, one considers an appropriate number of energy levels of the molecule of interest. For getting the values of energies of levels and the radiative transition probabilities among the levels, one depends on the laboratory study of the molecule. To the best of our knowledge, no information about the spectroscopic study of TiH_2 is available in the literature.

We have optimized the molecule TiH_2 with the help of GAUSSIAN 2009, where B3LYP method and cc-pVtz basis set are used, and obtained the values of rotational and centrifugal distortion constants (Table 1), and of the electric dipole moment. The TiH_2 is asymmetric top molecule with the Ray parameter $\kappa = -0.6164$. It is a planar molecule having C_{2v} symmetry and electric dipole moment $\mu = 2.792$ Debye along the b -axis of inertia. The bond length Ti-H is ~ 1.7077 Å and the angle H-Ti-H is $\sim 111.9^\circ$.

Owing to one-half value of spin of each of the two hydrogen atoms, the TiH_2 has two distinct species: (i) ortho (with parallel spins) and (ii) para (with anti-parallel spins). These two species behave as if they are two distinct molecules, as there are no transitions between them. Since the kinetic temperature in a cosmic object, where molecules are found, is few tens of Kelvin, we are concerned with the rotational levels in the ground vibrational and ground electronic states.

Using the values of rotational and centrifugal distortion constants, we have obtained energies of rotational levels. For each of the ortho- TiH_2 and para- TiH_2 , 40 rotational levels are shown in Figures 1 and 2, respectively. These levels are connected through radiative and collisional transitions.

Using the values of rotational and centrifugal distortion constants, and of electric dipole moment, the radiative transition probabilities (Einstein A -coefficients) are calculated. The radiative transitions are governed by some selection rules, derived on the basis of quantum mechanics. There are 89 radiative transitions among the ortho levels and 88 transitions among the para levels. The values of Einstein A -coefficients are rather large as compared

to those of a molecule, in general. For example, out the above transitions, 85 ortho and 83 para transitions have Einstein A -coefficient larger than 10^{-5} s^{-1} . The Einstein A -coefficient get value up to 1.1 s^{-1} .

Though the collisional transitions are not governed by any selection rules, but the computation of collisional rate coefficients is the most difficult task in the study of cosmic molecules. The collision partner is generally taken as the most abundant molecular hydrogen H_2 . When the collisional rate coefficients are not available, it is a common practice to use some scaling law for their calculation. We have calculated the collisional rate coefficients by using a scaling law⁴. They satisfy the condition that they do not produce any kind of anomalous phenomenon from their own. The collisional rate coefficients are of the order of $10^{-11} \text{ cm}^3 \text{ s}^{-1}$ or smaller. They are, in general, smaller than $10^{-11} \text{ cm}^3 \text{ s}^{-1}$.

For the known values of radiative and collisional transition probabilities, for each species, we have solved the set of statistical equilibrium equations coupled with the equations of radiative transfer. In the model⁵, the external radiation field, impinging on the volume element, generating the lines, is the cosmic microwave background (CMB) only, which corresponds to the background temperature $T_{bg} = 2.73 \text{ K}$. The parameter γ is expressed as $\gamma = n_{mol}/(dv_r/dr)$, where n_{mol} is the density of TiH_2 and (dv_r/dr) the velocity gradient in the cosmic object.

The set of equations is non-linear and is solved through iterative procedure, where the initial population densities of the levels are taken as the thermal ones. In order to include a large number of cosmic objects, where titanium dihydride may exist, we have considered wide ranges of physical parameters. The density of molecular hydrogen, n_{H_2} , is taken from 10^2 to 10^7 cm^{-3} , the kinetic temperature T is taken as 10, 20, 30, 40, 60, 80, 100 K. Two values of the parameter γ are taken as 5×10^{-7} and $5 \times 10^{-6} \text{ cm}^{-3} (\text{km/s})^{-1} \text{ pc}$. The abundance of TiH_2 in some cosmic object is expected to be large enough and these values of γ are quite reasonable.

For the kinetic temperatures considered here, the reliable results may be for the transitions among the levels up to $\sim 100 \text{ cm}^{-1}$. For these levels, there are 14 ortho and 16 para transitions. The brightness temperatures T_B of the lines are calculated by using the population densities of levels obtained by solving the set of equations. Except two transitions, $1_{11} - 0_{00}$ and $2_{02} - 1_{11}$ (both belonging to the para species), other 28 transitions are found to have low brightness temperature T_B , which is nearly equal to the temperature of the CMB (2.73 K). The brightness temperatures of the transitions $1_{11} - 0_{00}$ and $2_{02} - 1_{11}$ are shown in Figure 3. For low densities, the brightness temperature is equal to the CMB temperature. There is no formation of spectral line.

For the formation of a spectral line, there should be non-local thermal equilibrium (NLTE) in the object. For the NLTE, the collisional transition probabilities are comparable to the radiative transition probabilities. In Figure 3, the NLTE starts around the density of 10^5 cm^{-3} . This value of density is quite large as compared to that found ($\sim 10^4 \text{ cm}^{-3}$) in a cosmic object having molecules. It may be interpreted that the probability of the detection of TiH_2 in the ISM is low, whereas the probability of its formation is quite large.

It may finally be concluded that owing to the large values of Einstein A -coefficients, the detection of TiH_2 in the ISM is less probable.

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Table 1. Rotational and centrifugal distortion constants in MHz.

Constant	Value	Constant	Value
A	2.8589602×10^5	Φ_J	$2.037108491 \times 10^{-3}$
B	1.2520818×10^5	Φ_{JK}	$-1.928681064 \times 10^{-2}$
C	8.707408×10^4	Φ_{KJ}	$-1.946479675 \times 10^{-2}$
Δ_J	6.004343468	Φ_K	$5.110638046 \times 10^{-1}$
Δ_{JK}	-4.186548023×10^1	ϕ_J	$1.014000418 \times 10^{-3}$
Δ_K	2.549058853×10^2	ϕ_{JK}	$-3.557138924 \times 10^{-3}$
δ_J	2.465123434	ϕ_K	$1.085768474 \times 10^{-1}$
δ_K	2.332384340		

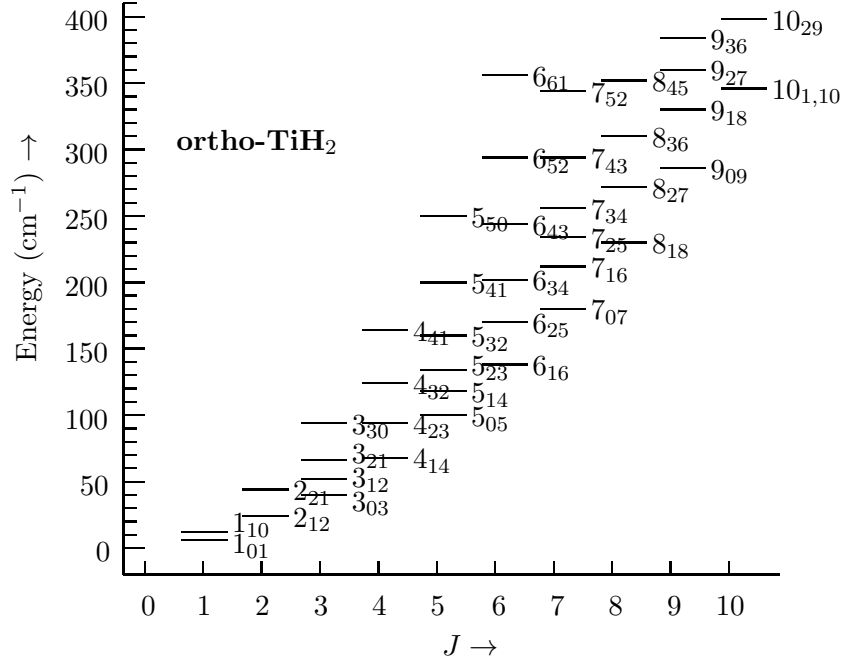


Figure 1: Energy level diagram for 40 levels of ortho-TiH₂.

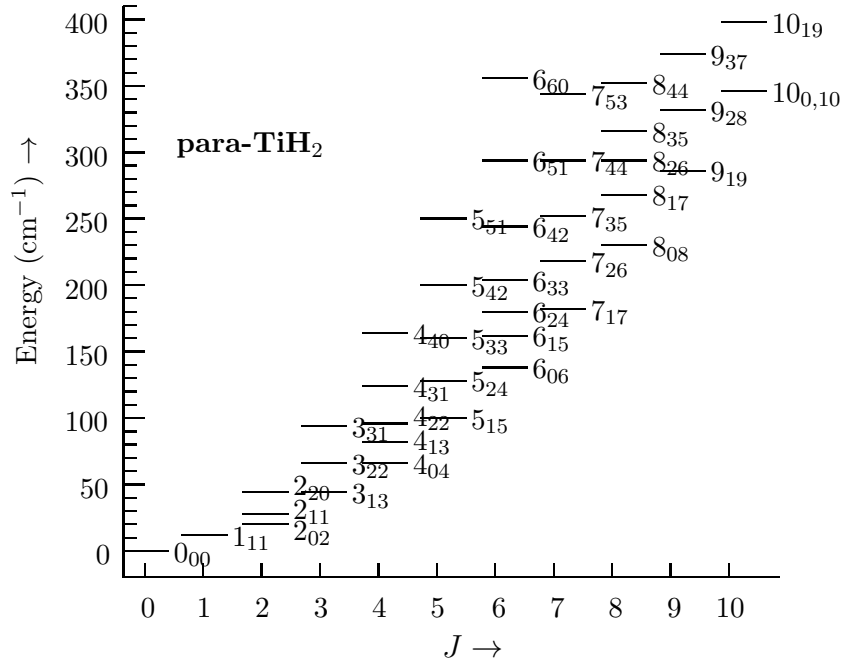


Figure 2: Energy level diagram for 40 levels of para-TiH₂.

Figure 3: Variation of brightness temperature T_B (K) versus hydrogen density n_{H_2} for seven values of kinetic temperature T (written on the top) for $1_{11}-0_{00}$ and $2_{02}-1_{11}$ transitions (written on the left) of TiH_2 . Solid line is for $\gamma = 5 \times 10^{-6} \text{ cm}^{-3} (\text{km/s})^{-1} \text{ pc}$, and the dotted line for $\gamma = 5 \times 10^{-7} \text{ cm}^{-3} (\text{km/s})^{-1} \text{ pc}$.

